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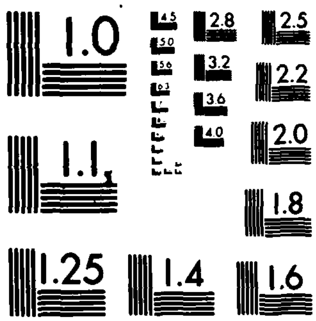

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by

M.A. STEPHENS

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DEPARTMENT OF STATISTICS
Stanford University
Stanford, California

FURTHER EXAMINATION OF SIMULATED PERCENTAGE POINTS

By

M.A. Stephens
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1. Introduction.

In a previous report, Juritz, Juritz and Stephens (1981) discussed methods of obtaining percentage points of distributions by Monte Carlo studies, either by using one long run, or using the average of several smaller runs. The single run has certain advantages--in particular, less bias. The two methods were illustrated using Monte Carlo studies. In this follow up, the comparison is continued, using as illustrations the normal and exponential distributions, for which exact values of order statistics can easily be found. An amalgamation of the earlier report and this one is now published in Juritz, Juritz and Stephens (1983).

2. The Single-Sample Method.

We first summarize previous results. Let $f(x)$ be the probability density function of a continuous random variable X, let $0 < p < 1$, and let ξ_p denote the (100p)th percentile of X. Let the order statistics of a random sample of size n drawn from $f(x)$ be $X_{(1)} < X_{(2)} < \cdots < X_{(n)}$. Suppose $k = [np] + 1$, where $[m]$ denotes the largest integer less than or equal to m; $X_{(k)}$ is the usual estimator of ξ_p, from the run of n Monte Carlo values of X. Furthermore, for X continuous, the random interval $(X_{(r)}, X_{(s)})$ with $r < s$ covers ξ_p with probability $\pi(r,s,n,p)$ given by

$$\text{Prob}(X_{(r)} \le \xi_p < X_{(s)}) = \pi(r,s,n,p) = \sum_{i=r}^{s-1} \binom{n}{i} p^i (1-p)^{n-i} ,$$

where

$$p = \text{Prob}(X \le \xi_p) .$$

Let $w = \{np(1-p)\}^{1/2}$, and let z_γ denote the (100γ)th percentile of the standard normal distribution. Then with

(1) $$r = -wz_\gamma + np + \frac{1}{2} \quad \text{and} \quad s = wz_\gamma + np + \frac{1}{2} ,$$

where $\gamma = 1-\alpha/2$, the interval $I_s = (X_{(r)}, X_{(s)})$ gives a confidence interval for ξ_p at level $100(1-\alpha)\%$, since $\pi(r,s,n,p)$ is then $1-\alpha$ (approximately, but to high accuracy).

3. <u>The Multi-Sample Method</u>.

In this method, proposed by Schafer (1974), c runs with m repetitions $(n = cm)$ are made. For each run the sample percentile $X_{(\ell)}$, where $\ell = [mp] + 1$, estimates ξ_p. Let $X_{(\ell)}$ be called X_p, and let the c values of X_p be $X_{p1}, X_{p2}, \ldots, X_{pc}$; the percentile ξ_p is estimated by the average

(2) $$\bar{X}_p = \frac{1}{c} \sum_{i=1}^{c} X_{pi}$$

and the variance σ^2 of $X_p = X_{(\ell)}$ is estimated by

(3) $$S^2 = \sum_{i=1}^{c} (X_{pi} - \bar{X}_p)^2/(c-1) \ .$$

The multi-sample confidence interval is

(4) $$I_m \equiv (\bar{X}_p - t_{1-\alpha/2} S c^{-1/2},\ \bar{X}_p + t_{1-\alpha/2} S c^{-1/2}) \ ;$$

this is a confidence interval for ξ_p with approximate confidence probability $1-\alpha$, where $t_{1-\alpha/2}$ is the upper $100(1-\alpha/2)^{th}$ percentile of Student's t with $c-1$ degrees of freedom. The number of runs must be chosen to give a good estimate of the standard deviation.

4. Bias in Point Estimates.

The question now arises: is it best to make c runs and then take the mean $\bar{X}_p$, as the point estimate $\hat{\xi}_p$ of ξ_p, or to make one large run and take $X_{(k)}$ as the estimate? In both cases the point estimates are biased in finite samples.

Let $Q(\cdot)$ be the inverse function of the parent population, and let $Q^{(i)}(\cdot)$ be its i^{th} derivative. In the previous report results in David (1970) were used to show that, to terms of order $1/n$,

(5) $$E(X_{(k)}) = Q(p) + \frac{1-p-\varepsilon_1}{n+1} Q^{(1)}(p) + \frac{p(1-p)}{2(n+2)} Q^{(2)}(p) \ ,$$

where $\varepsilon_1 = np - [np]$.

When several samples are used, the estimate $\hat{\xi}_p$ of ξ_p is $\bar{X}_p = \bar{X}_{(\ell)}$ where ℓ is $[mp] + 1$. Then to order $1/m$,

$$(6) \qquad E(\bar{X}_{(\ell)}) = E(X_{(\ell)}) = Q(p) + \frac{1-p-\varepsilon_2}{m+1} Q^{(1)}(p) + \frac{p(1-p)}{2(m+2)} Q^2(p)$$

where $\varepsilon_2 = mp - [mp]$.

In most practical applications, for the sample sizes and p-values one would use in estimating percentiles accurately from Monte Carlo samples, both ε_1 and ε_2 would be zero. Then from (5) and (6) the bias of the single sample estimate is smaller than that of the multi-sample estimate by a factor of size approximately c.

5. Expected Lengths of Confidence Intervals.

It is worthwhile to compare the expected lengths of the confidence intervals (CI) for ξ_p, obtained by the two methods. CI for Monte Carlo points are rarely given, although they would be useful when using such points to check other methods of obtaining points, for example, by curve-fitting to the moments. For the single-sample case the CI is $I_s \equiv (X_{(r)}, X_{(s)})$, where r and s are given in (1), and this is very easily found. The expected length L_s of I_s is $E(X_{(s)} - X_{(r)})$; we have

$$L_s = Q(p_s) - Q(p_r) + O(1/(n+2)) ,$$

where $p_s = s/(n+1)$ and $p_r = r/(n+1)$. To order $n^{-1/2}$ this is, using (5)

$$(7) \qquad L_s = Q^{(1)}(p)\, 2\, z_{1-\alpha/2}\{p(1-p)\}^{1/2}/n^{1/2} .$$

For the multi-sample method the CI is I_m given in (4). For its expected length we need $E(S/c^{1/2})$; $E(S^2)$ is $\mathrm{Var}(X_{(\ell)})$, which for the normal case can be found quite accurately using the method of Davis and Stephens (1978). However, for large samples, as here, we can use (David, 1970, p. 65)

$$(8) \qquad \sigma^2 = \mathrm{Var}\{X_{(\ell)}\} = \frac{p_\ell q_\ell}{m+2} \{Q^{(1)}(p_\ell)\}^2 + 0\{1/(m+2)^2\} ,$$

where $p_\ell = \ell/(n+1)$ and $q_\ell = 1-p_\ell$. Thus, to order $1/n$, the variance σ^2/c of the multi-sample estimate $\bar{X}_p$ is

$$(9) \qquad \mathrm{Var}(\bar{X}_p) = \mathrm{Var}(\bar{X}_{(\ell)}) = E\left\{\frac{S^2}{c}\right\} = \frac{p(1-p)}{n} \{Q^{(1)}(p)\}^2$$

and the expected length L_m of the confidence interval I_m is, to order $n^{-1/2}$

$$(10) \qquad L_m = 2\{p(1-p)\}^{1/2} Q^{(1)}(p) t_{1-\alpha/2}/n^{1/2} .$$

This is the same as L_s but with $t_{(1-\alpha/2)}$ replacing $z_{(1-\alpha/2)}$. Thus, since c will usually be quite small, L_m will be larger than L_s; also the accuracy of I_m may be poor since it depends on the normal distribution for the values $X_{p1}, X_{p2}, \ldots, X_{pc}$, and this does not hold well for extreme order statistics. There is also a difference in the nature of the confidence intervals: the interval I_m obtained by the multi-sample method will have endpoints equally spaced about the estimate $\bar{X}_{(\ell)}$, while I_s is designed so that the endpoints have estimated

significance levels equally spaced about p. For many uses of confidence intervals the second property may well be the more desirable.

6. Examples.

6.1. Point estimates.

The comparison between the single-sample and the multi-sample method can be illustrated very well by the normal and exponential distributions, for which expected values of order statistics $m_k \equiv E\{X_{(k)}\}$ are extensively tabulated or can be easily calculated.

The normal distribution. Consider the estimation of $\xi_{.95}$, the 95th percentile of the normal distribution which has a true value of 1.6449. Table 1 gives values of m_k for the relevant order statistics, (from Harter, 1961, for $n \leq 400$) and the bias in the estimates. Table 1 can be used as follows. Suppose the choice of estimator is between $n = 400$ replicates in one run, or $c = 4$ runs of $m = 100$ replicates. For the multi-sample case, the estimator is $\overline{X}_{(96)}$, with expected value 1.6872; for one sample, the estimator $X_{(381)}$ has expected value 1.6553. The bias is reduced, as expected, by a factor of about 4. For larger values of n the first terms in (5) give an excellent approximation to m_k; for example, for $n = 400$, $k = 381$, (5) gives 1.6552 to compare with the exact value 1.6553. Another very good approximation is that given by Blom (1958): $m_k \doteq Q(Z_k)$ where $Z_k = (k-0.375)/(n+0.25)$; for $n = 400$, $k = 389$ Blom's formula gives 1.6543. Equation (5) is marginally more accurate so we use it for values of n greater than 400 (the limit of Harter's (1961) table).

Suppose, for a second example, the choice is between one run with $n = 10000$ replicates and $c = 10$ runs of $m = 1000$ replicates, and suppose the estimate is required for $\xi_{.975}$, which has a true value 1.9600. Table 1, in the second part, shows that the bias for the single-sample case is 0.0007, approximately one-tenth that of the bias (0.0074) in the multi-sample case, as expected.

The table also shows cases where the multi-sample bias can be lower than the single-sample bias. For example, the bias using $m = 500$ when estimating $\xi_{.975}$ is, from the second part of Table 1, -0.0026; if $c = 2$, the single-sample would have 1000 samples for which the bias is 0.0074. However, if a confidence interval were required for $\xi_{.975}$, it would be foolish to base the variance estimate on only 2 runs; and for $c = 4$ or more the bias is again smaller using only one large sample. The anomaly arises only because when $m = 500$, $p = .975$, the quantity mp is not an integer, and it happens then that m_{488} gives a bias smaller than the bias in m_{976} for $n = 1000$; it is also negative. In practice the multi-sample bias will be smaller only in somewhat contrived examples such as the above.

6.2. Confidence intervals.

(a) Accuracy of the single-sample C.I.

Table 1 also gives the values of r and s used to calculate I_s, the confidence interval given by the single-sample method, L_s, the exact length of I_s, and the length as estimated from (7); it can be seen that (7) gives a slightly smaller length than the correct L_s in smaller samples.

(b) Accuracy of the multi-sample C.I.

In determining the accuracy of L_m above we do not use the approximation (8) for the variance of an order statistic. However, the approximation (10) for L_s makes use of (8), and this is an approximation which cannot easily be checked accurately, since exact tables of the variance of $X_{(k)}$ do not exist for large samples; (9) above gives an approximation to order $1/n$, and Davis and Stephens (1978) give a good approximation. However, we have taken Monte Carlo samples to examine confidence intervals further, and to see the variations of estimates in practice.

A test will consist of c runs of m, to give the multi-sample results, and one run of $n = cm$ obtained by combining the c runs into one. In the study to be reported, c was taken as 10. For each test, the sample mean $\bar{X}_p$ and the standard deviation S (equations (2) and (3) above) of the 10 estimates of $\xi_{.95}$, based on m values, were calculated, as they would be in the multi-sample method, and the 95% confidence interval I_m found from (4). In the top half of Table 2 these values are given for two values of m, 100 and 500. The bias in the estimate and the length of the confidence interval are also given.

In the bottom half of the table are recorded the results for the single-sample method. Since 6 tests have been made, the standard deviation of X_p for this method can be estimated in the usual way. It can be seen from the table that the Monte Carlo estimates of bias are around the values given in Table 1; also the sample variances of the estimates agree, to within sampling fluctuations, with values calculated from equation (9). The lengths of the confidence intervals are roughly the same by each method, as predicted in Section 5; S is much larger, say, for a sample of $m = 100$ than it is for

a sample of $n = 1000$, but in calculating the confidence interval it must be divided by $\sqrt{10}$, and this brings the length of the intervals for the multi-sample method (top half of Table 2) to roughly the same size as those for the single-sample method (bottom half of Table 2). Note that there appears to be some correlation between the length of I_m and that of I_s.

Results for $p = 0.975$ are of the same pattern, although they are not given here. So also are the results of similar tests for $n = 2000$, and 10000.

6.3. The exponential distribution.

Table 3 gives results for the exponential distribution corresponding to those in Table 1 for the normal distribution. Again the bias for a multisample estimate must be given by entering the table at the value of m, and that for the single-sample estimate is given by entering at n. Thus for an estimate of $\xi_{.95}$, with $m = 500$ and $c = 10$, say, the bias is .0212, but for $n = cm = 5000$ the bias in .0021, almost exactly one-tenth. The exact expected length of a single-sample 95% confidence interval is given in column 9; the value of this length approximated by (7) is in the last column. The approximation given by (7) is quite accurate even for sample sizes which would be considered small in Monte Carlo sampling (for example, 500).

6.4. The uniform distribution.

For estimates of ξ_p for the uniform distribution on $[0,1]$, comparisons between the two methods are straightforward. For simplicity consider the case where mp is an integer. Then for the single-sample method, $k = np+1$ and for the multi-sample method $\ell = mp+1$.

Then $E(X_{(k)}) = (np+1)/(n+1)$ and $E(\overline{X}_p) = E(\overline{X}_{(\ell)}) = E(X_{(\ell)}) = (mp+1)/(m+1)$. The bias, for the single sample estimate is $(np+1)(n+1)-p = (1-p)/(n+1)$; for the multisample estimate it is $(1-p)/(m+1)$. The bias in the estimates is always positive. The variance of $X_{(\ell)}$ is $V = \{m(mp+1)(1-p)\}/\{(m+1)^2(m+2)\}$, which is, to order $1/m$, $V = p(1-p)/m$. Thus the variance of $\overline{X}_{(\ell)} = \overline{X}_p$, which is V/c, is $p(1-p)/n$, to order $1/n$. This is also, to the same order, the variance of $X_{(k)}$ in one large run of size n. Thus the C.I. for the percentile ξ_p will be approximately the same length when obtained by either the multi-sample method or the single-sample method, but the bias in the estimate is reduced, as in earlier examples, by a factor of approximately c using the single-sample method.

Further remarks. Krutchkoff (1980) and Reynolds (1980) have discussed the parallel question of estimating the tail probability of a distribution corresponding to a particular value of x. These authors have also suggested that it is better to use a single sample, rather than several runs of a smaller size, to estimate this probability.

Table 1

Expected values of order statistics from the normal distribution, used in estimates and confidence intervals for ξ_p.

n	k	m_k	bias x 10^4	r	m_r	s	m_s	L_s:Exact Expected C.I. Length	Expected C.I. Length From (7)
			$p = 0.95$; True $\xi_p = 1.6449$						
100	96	1.6872	423	92	1.3656	100	2.4986	1.133	0.823
400	381	1.6553	104	372	1.4652	390	1.9361	0.471	0.413
500	476	1.6531	82	466	1.4821	486	1.8934	0.411	0.370
1000	951	1.6490	41	937	1.5254	965	1.8046	0.279	0.262
5000	4751	1.6457	8	4721	1.5900	4781	1.7070	0.117	0.117
10000	9501	1.6453	4	9458	1.6049	9544	1.6885	0.084	0.083
100000	95001	1.6449	0	94866	1.6319	95136	1.6581	0.026	0.026
			$p = 0.975$; True $\xi_p = 1.96004$						
100	98	1.9464	-136	95	1.5912	-	-	-	-
400	391	1.9787	187	385	1.7632	397	2.3690	.606	.523
500	488	1.9574	-26	481	1.7606	495	2.2852	.525	.461
1000	976	1.9674	74	966	1.8175	986	2.1816	.364	.331
5000	4876	1.9614	14	4854	1.8910	4898	2.0433	.152	.148
10000	9751	1.9607	7	9720	1.9101	9782	2.0168	.107	.105
100000	97501	1.9600	0	97404	1.9437	97598	1.9769	.033	.033

Table 2

Estimates from 6 tests of 10 Monte Carlo samples; $p = .95$, true $\xi_p = 1.645$

1. Multi Sample Results.

$c = 10$, $m = 100$. St. Dev. σ of $X_{(\ell)}$, from (8) = 0.210

Test	Estimate $\bar{X}_p$	Bias $\times 10^3$	S	C.I. Limits (Equation 4) Lower	C.I. Limits (Equation 4) Upper	I_m C.I. Length
1	1.794	149	.220	1.637	1.952	.315
2	1.792	147	.134	1.697	1.888	.192
3	1.676	31	.182	1.546	1.806	.260
4	1.668	23	.133	1.572	1.763	.190
5	1.685	40	.214	1.533	1.838	.305
6	1.589	-56	.246	1.413	1.765	.352

Average Bias $\times 10^3$ = 56: Expected bias = 42.3

$c = 10$, $m = 500$. St. Dev. σ of $X_{(\ell)}$, from (8) = 0.094

Test	Estimate $\bar{X}_p$	Bias $\times 10^3$	S	C.I. Limits (Equation 4) Upper	C.I. Limits (Equation 4) Lower	I_m C.I. Length
1	1.644	-1	.098	1.574	1.715	.141
2	1.667	22	.113	1.586	1.748	.162
3	1.640	-5	.113	1.559	1.722	.163
4	1.688	43	.064	1.642	1.734	.092
5	1.692	47	.105	1.617	1.767	.150
6	1.645	0	.087	1.583	1.707	.124

Average Bias $\times 10^3$ = 18: Expected bias = 8.2

2. Single Sample Results.

$n = 1000$

Test	Estimate X_p	Bias $\times 10^3$	C.I. Limits Lower	C.I. Limits Upper	I_s C.I. Length
1	1.714	69	1.589	1.897	.308
2	1.721	76	1.627	1.822	.195
3	1.593	-52	1.490	1.699	.209
4	1.687	42	1.529	1.822	.293
5	1.612	-33	1.531	1.775	.244
6	1.554	-91	1.427	1.669	.242

Average Bias $\times 10^3$ = 1.8: Expected bias = 4.1

Estimate S of σ from 6 values X_p: .070

$\hat{\sigma}$ from (8) : .067

$n = 5000$

Test	Estimate X_p	Bias $\times 10^3$	C.I. Limits Lower	C.I. Limits Upper	I_s C.I. Length
1	1.635	-10	1.581	1.698	.117
2	1.648	3	1.587	1.713	.126
3	1.638	-7	1.584	1.695	.111
4	1.673	28	1.626	1.746	.120
5	1.687	42	1.602	1.750	.148
6	1.639	-6	1.591	1.700	.109

Average Bias $\times 10^3$ = 9: Expected bias = 0.8

Estimate S of σ from 6 values X_p: .022

$\hat{\sigma}$ from (8) : .030

Table 3

Expected values of order statistics from the exponential distribution, used in estimates and confidence intervals for ξ_p.

$p = .95$; True $\xi_p = 2.9957$

n	k	m_k	bias x 10^4	r	m_r	s	m_s	L_s:Exact Expected C.I. Length	Expected C.I. Length From (7)
100	96	3.1040	1083	92	2.4695	100	5.1874	2.718	1.802
400	381	3.0222	265	372	2.6428	390	3.6410	.998	.866
500	476	3.0169	212	466	2.6746	486	3.5413	.867	.772
1000	951	3.0063	106	937	2.7572	965	3.3387	.582	.543
2000	1901	3.0010	53	1882	2.8262	1920	3.2129	.387	.383
5000	4751	2.9978	21	4721	2.8843	4781	3.1259	.242	.242
10000	9501	2.9968	11	9458	2.9142	9544	3.0868	.173	.171
100000	95001	2.9958	1	94866	2.9692	95136	3.0232	.054	.054

$p = .975$; True $\xi_p = 3.6889$

n	k	m_k	bias x 10^4	r	m_r	s	m_s	L_s:Exact Expected C.I. Length	Expected C.I. Length From (7)
100	98	3.6874	-15	95	2.9040	-	-	-	-
400	391	3.7410	521	385	3.2517	397	4.7366	1.485	1.221
500	488	3.6896	72	481	3.2451	495	4.5095	1.264	1.093
1000	976	3.7095	206	966	3.3673	986	4.2339	.867	.773
2000	1951	3.6992	103	1937	3.4501	1965	4.0316	.582	.547
5000	4876	3.6930	41	4854	3.5303	4898	3.8874	.357	.346
10000	9751	3.6909	20	9720	3.5738	9782	3.8236	.250	.248
100000	97501	3.6891	2	97404	3.6510	97598	3.7287	.078	.077

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